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Thermal switch using controlled capillary transition in heterogeneous nanostructures

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ABSTRACT

The development of a nanoscale thermal switch is a crucial step toward advanced thermal management systems including future thermal logic gates and computers. This study demonstrates a new nanoscale thermal switch mechanism using controlled, morphological transition from adsorption to capillary state in a novel gas-filled nanostructure, i.e., a nanogap with controllable nanoposts on one surface only. The degree of thermal switch, S, at given gas pressures are predicted using Ar-filled Pt-based nanostructures and Non-Equilibrium Molecular Dynamics (NEMD) simulation combined with Grand Canonical Monte Carlo (GCMC) simulation. It is found that S increases by increasing the height of the nanoposts and temperature difference across the nanostructure, and decreasing the interpost spacings, with the maximum degree of switch, $S_{max} \sim 45$ and ~ 170 for $\Delta T = 10$ K and 60 K, respectively, for the nanogap size of 5 nm. It is also observed that a stronger solid-fluid surface interaction results in a wider switch operating temperature window.

1. Introduction

A thermal switch is a system which maximizes ("on" mode) or minimizes ("off" mode) a thermal transport on demand, and it critically serves as a thermal management system in various applications including energy dissipation and thermal stabilization in miniaturized devices [1,2], spacecraft [3], energy scavenging [4,5], and the realization of thermal circuits/logic gates [6]. The efficient thermal switch needs an outstanding contrast between thermal transport in "on" and "off" modes with a reasonable response time, i.e., good thermal conductor in "on" mode and thermal insulator in "off" mode. To demonstrate the effectiveness of the switching, the degree of the thermal switch, S, is defined as the ratio of the "on" mode to "off" mode heat flux, given as

$$S = \frac{|\boldsymbol{q}_{on}|}{|\boldsymbol{q}_{off}|}, \tag{1}$$

where $|\boldsymbol{q}_{on}|$ and $|\boldsymbol{q}_{off}|$ are the heat fluxes in "on" and "off" modes, respectively.

To improve the degree of thermal switch, various thermal switching mechanisms have been explored using nonlinear conduction, convection, radiation, or the combination of them. The conduction-based thermal switch primarily benefits from the mechanical movements of thermal switching mechanisms using temperature-controlled and non-temperature controlled actuators. Temperature-controlled actuating approaches include methods based on Differential Thermal Expansion (DTE) [7–11], as well as the characteristics of shape memory alloys [3], bi-metalic materials [12], three-terminal graphene nanoribbons [13], liquid-metal phase-change-based volume expansion [14–18], or different thermal accommodation coefficient on heterogeneous surfaces of the nanogaps [19]. Thermal switch demonstrations by non-temperature-controlled actuating approaches include gas pressure control in gas-gap setups [4,5,20–23], employing electrostatic actuation [24], liquid water morphological change on Teflon coated substrates [25], dielectric liquids [26], temperature-dependent oscillation of the ferromagnetic materials [27], and carbon nanotube deflection by electrostatic loads [28]. Nonlinear-convection-based thermal switches have been also explored by approaches based on heat pipes controlled by shape memory alloys [29], double-loop heat pumps [30], and three-internally-layered setups with one hydrophilic and one hydrophobic surface [31]. Nonlinear radiation achieved by controllable emissivity [32,33], near-field radiation [34,35], thermoelectricity [36], magnetic field between the heat source and sink [37], or VO_2 insulator-to-metal phase transition [2] can also offer thermal switching mechanisms. Applying recent molecular-level theoretical studies explore another branch of thermal switching demonstrations based on quantum thermal shuttling between the source and the sink [38],

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temperature-biased quantum junctions [39,40], and three-terminal Coulomb-coupled quantum dots [41].

In gas-filled nanostructures, the gas prematurely turns into liquid state, i.e., adsorption-capillary transition, below the saturation pressure at given temperature [42,43]. This transition is associated with the gas pressure, temperature, surface-fluid interaction, and structural parameters [44]. This transition between the states includes not only the morphological changes, i.e., adsorption to capillary, but also thermal properties such as the low thermal conductivity of gas to the high thermal conductivity of liquid. This significant gas thermal conductivity change between two states could potentially lead to the thermal switching mechanism, but it has not been fully realized yet.

In this study, we examine an adsorption-capillary-transition-controlled thermal switch in a nanogap with movable nanopost structures where the nanogap surfaces also operate as the heat source and the heat sink. The switch performance is demonstrated with controlled nanopost height on one surface only, using Grand Canonical Monte Carlo (GCMC) simulation combined with Non-Equilibrium Molecular Dynamics (NEMD) simulations. The heat fluxes across the gas-filled nanostructures and degree of thermal switch are predicted as functions of operating temperature, nanostructure geometries, and solid-fluid interaction parameters. Optimal designs and operating conditions are also discussed. This new class of thermal switching mechanism is compatible with the thermal diode and transistor mechanisms [19,45] and is capable of achieving $S \sim 170$ in an order of 10 ns.

2. Working principle

The adsorption-capillary-transition-controlled thermal switch stems from a large thermal transport contrast between the adsorption and capillary states in heterogeneous nanostructures. The adsorption-capillary transition in nanostructures is related to the surface tension of fluid, gas pressure, temperature, and the size of the nanostructures [42,43]. To further control the adsorption-capillary transition, a heterogeneous nanostructure aiming at designing the thermal switch, i.e., Ar-gas filled Pt-based nanogap with nanoposts on one side only, is employed as shown in Fig. 1 (a)–(c). Detailed discussions on the adsorption-capillary transition in Ar-filled heterogeneous nanostructure are found in previous work [44], but this study primarily focuses on the thermal switching mechanism due to the adsorption-capillary transition. At high temperature and low gas pressure, Ar fills the nanogap as gaseous state, i.e., adsorption state. The thermal conductivity across the Ar-gas filled nanostructure is relatively small due to the low number density of gas and large interfacial resistance between the gas and solid, i.e., Thermal Accommodation Coefficient (TAC). This low thermal conductivity serves as the "off" mode.

The gas thermal conductivity across the nanostructure is given as [46,47]

$$\langle k_{f,t} \rangle = \langle k_{f,fm} \rangle \left(1 + \frac{4}{15} \frac{1}{Kn} \frac{a_{T,1} a_{T,2}}{a_{T,1} + a_{T,2} - a_{T,1} a_{T,2}} \right)^{-1}, \tag{2}$$

where Kn is the Knudsen number and $a_{T,1}$ and $a_{T,2}$ are the TACs. In free-molecular region ($Kn > 10$), the gas thermal conductivity, $\langle k_{f,fm} \rangle$, is given as [48]

$$\langle k_{f,fm} \rangle = \frac{p\left(c_{v,f} + \frac{R_g}{2}\right)}{a_{T,1}^{-1} + a_{T,2}^{-1} - 1} (2\pi M R_g T)^{-1/2} L_z, \tag{3}$$

where p is the gas pressure, $c_{v,f}$ is the heat capacity, R_g is the ideal gas constant, M is the molecular mass of the gas, T is the gas temperature, and L_z is the nanogap size.

For the "on" mode, a higher thermal conductivity across the capillary-condensed Ar in a heterogeneous nanostructure is achieved by inserting nanoposts into the nanogap as shown in Fig. 1(c). The higher thermal conductivity for the condensed Ar in the nanostructure primarily stems from the higher Ar number density and phononic energy transfer, given as [49,50]

$$k_f = \frac{3R_g}{N_A^{1/3}} \frac{\rho_f^{1/6}}{M^{2/3}} \left(\frac{c_{p,f}}{c_{v,f}} \frac{1}{\kappa_f} \right)^{1/2}, \quad \kappa_f = \frac{1}{\rho_f} \frac{\partial \rho_f}{\partial p}\bigg|_T \tag{4}$$

where N_A is the Avogadro Number, ρ_f is the fluid density, and $c_{p,f}$ and $c_{v,f}$ are the specific heat at constant pressure and volume, respectively.

Note Ar is chosen here for the proof of concept with relatively well-studied potential in literature [51–54] and relatively smaller computational cost (monatomic gas). However, this working principle can be extended to the different types of fluid as long as the gas is condensable at given temperature and pressure, for example, water at ambient pressure and temperature.

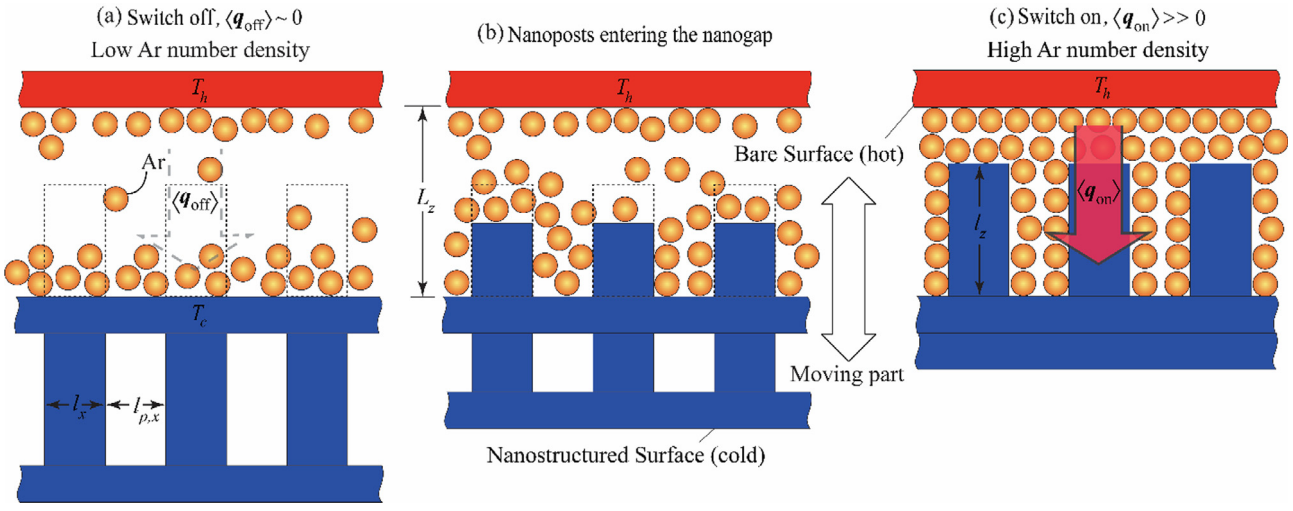

Fig. 1. Schematic drawing of adsorption-capillary-controlled thermal switch at given pressure and temperature. (a) Nanoposts are located outside the nanogap, aiming at delaying the capillary transition (gas state only) for switch "off" mode. (b) A snapshot of the intermediate stage between switch "on" and "off" under given gas pressure. (c) Nanoposts are mechanically moved into the nanogap to facilitate capillary transition (condensation) at the given temperature, thereby resulting in switch "on" mode. The dimensions for the nanogap and nanoposts are also shown.